Journal of Mathematics Research; Vol. 14, No. 2; April 2022
ISSN 1916-9795 E-ISSN 1916-9809
Published by Canadian Center of Science and Education

A Mixed Volume Element Modified With Characteristic Fractional Step Difference Method for the Compressible Multicomponent Displacement and Its Numerical Analysis

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Received: October 3, 2021 Accepted: January 30, 2022 Online Published: March 3, 2022

doi:10.5539/jmr.v14n2p6 URL: https://doi.org/10.5539/jmr.v14n2p6

Abstract

A three-dimensional compressible problem with different components is fundamental in numerical simulation of enhanced oil recovery. The mathematical model consists of a parabolic equation for the pressure and a convection-diffusion system for the concentrations. The pressure determines Darcy velocity and plays an important role during the whole physical process. A conservative mixed volume element is used to discretize the flow equation, and improves the computational accuracy of Darcy. The concentrations are computed by the modified characteristic fractional step difference scheme, thus numerical dispersion and nonphysical oscillations are eliminated. The whole three-dimensional computation is accomplished effectively by solving three successive one-dimensional problems in parallel, where the speedup method is used and the work is decreased greatly. Based on the theory and special techniques of a priori estimates of partial differential equations, an optimal second error estimates in L^2-norm is concluded. This work concentrates on the model, numerical method and convergence analysis for modern oil recovery.

Keywords: three-dimensional compressible multicomponent, oil-water seepage displacement, mixed volume element, modified characteristic fractional step difference, second error estimates in L^2-norm

1. Introduction

An important tool is used usually in modern oil recovery that high-pressure pump drives water into oil reservoir and displaces the crude oil from production wells. The 3-D problem is studied carefully in this paper. In modern oil-gas development process, a new enhanced oil recovery (chemical oil recovery) technique is adopted to displace the remnant crude oil from oil reservoir. The compressibility of fluid and the multicomponent must be considered in numerical simulation of enhanced oil recovery, otherwise numerical simulation probably distorts the truth. Douglas and other researchers first put forward the mathematical model for a compressible miscible multicomponent flow, and discuss the method of characteristic finite element and the method of characteristic mixed finite element.

The mathematical model is defined by a nonlinear partial differential system with the initial-boundary conditions (Douglas & Roberts, 1983a; Ewing, 1983; Yuan, 1992,1993,1999, 2003, 2013):

$$d(c)\frac{\partial p}{\partial t} + \nabla\cdot\mathbf{u} = qX,t,\ X = (x,y,z)^T \in \Omega, t \in J = (0,T], \tag{1a}$$

$$\mathbf{u} = -a(c)\nabla p,\ X \in \Omega,\ t \in J, \tag{1b}$$

$$\phi(X)\frac{\partial c_\alpha}{\partial t} + b_\alpha(c)\frac{\partial p}{\partial t} + \mathbf{u}\cdot\nabla c_\alpha - \nabla\cdot(D\nabla c_\alpha) = g(X,t,c_\alpha),\ X \in \Omega, t \in J, \alpha = 1,2,\cdots,n_c. \tag{2}$$

Here $p(X,t)$ is the pressure, and $c_\alpha(X,t)$ is the αth concentration for $\alpha = 1,2,\cdots,n_c$. n_c is the number of components. Because of $\sum_{\alpha=1}^{n_c} c_\alpha(X,t) = 1$, only $n_c - 1$ components are independent. Let $c(X,t) = (c_1(X,t), c_2(X,t),\cdots,c_{n_c-1}(X,t))^T$ denote the concentration vector. $\phi(X)$ is the porosity, z_α is the αth compressibility coefficient, and $d(c) = \phi(X)\sum_{\alpha=1}^{n_c} z_\alpha c_\alpha$. $\mathbf{u}(X,t)$ is Darcy velocity. $\kappa(X)$ is the permeability, $\mu(c)$ is the viscosity and $a(c) = \kappa(X)\mu^{-1}(c)$. $b_\alpha(c) = \phi c_\alpha\{z_\alpha - \sum_{j=1}^{n_c} z_j c_j\}$.

$D = D(X)$ is the diffusion. The pressure $p(X, t)$ and the vector $c(X, t)$ should be computed.

Assume that no flow occurs at the boundary,

$$\mathbf{u} \cdot \gamma = 0,\ X \in \partial\Omega,\ (D\nabla c_\alpha - c_\alpha \mathbf{u}) \cdot \gamma = 0, X \in \partial\Omega, \alpha = 1, 2, \cdots, n_c - 1, \tag{3}$$

where γ is the outer normal vector to the boundary $\partial\Omega$.

Initial values:

$$p(X, 0) = p_0(X),\ X \in \Omega,\ c_\alpha(X, 0) = c_{\alpha,0}(X),\ X \in \Omega, \alpha = 1, 2, \cdots, n_c - 1. \tag{4}$$

Under the assumptions on periodic conditions, the characteristic numerical methods and their theoretical analysis are discussed for incompressible problems (Douglas, 1983b, 1986; Russell, 1985; Ewing, Russell & Wheeler, 1984). The composite methods, combining the characteristics and standard finite difference or finite element, could interpret the hyperbolic of convection-diffusion equation, eliminate numerical dispersion, reduce the truncation, and improve the computational stability and accuracy. For simulating the problem of modern enhanced (chemical) oil recovery well, the compressibility and multicompoment should be considered (Ewing, Yuan & Li, 1989; Yuan, Yang & Qi, 1998). Douglas and Yuan present the characteristics related methods, such as characteristic finite element, characteristic mixed element and characteristic fractional step difference, and give optimal error estimates in L^2-norm for the actual problem with periodic assumptions (Douglas & Roberts, 1983a; Yuan, 1992, 1993, 2001,2003). Finite volume element (Cai, 1991; Li & Chen, 1994) inherits the simplicity from the finite difference and the high accuracy from the finite element, preserves the conservative nature, thus becomes a powerful tool for solving the partial differential equations. Mixed finite element method could solve the pressure and Darcy velocity simultaneously (Raviart & Thomas, 1977; Douglas, Ewing & Wheeler, 1983c, 1983d), and improves the accuracy of Darcy. Finite volume element and mixed finite element are combined to give a new mixed finite volume element (Ewing, 1983; Russell, 1995; Weiser & Wheeler, 1988), and its computational efficiency is tested experimentally (Jones, 1995; Cai, Jones, Mccormilk & Russell, 1997). A frame work is concluded showing convergence analysis of mixed finite volume element for elliptic problems (Chou, Kawk & Vassileviki, 1998,1999,2000), and is applied in numerical simulation for a Darcy-Forchheimer flow problem (Pan & Rui, 2012; Rui & Pan, 2012).

The compressibility and the multicomponent are considered in simulating the physical displacement of enhanced oil recovery. The computational work is large-scaled on a three-dimensional region and a long time interval. Millions of variable nodes are involved, so some standard numerical methods are invalid. Then, an effective fractional step method is proposed (Ewing, 1983; Yuan, 2013; Shen, Liu & Tang, 2002). Peaceman and Douglas discuss the fractional step difference to solve a two-dimensional problem but argue the stability and convergence only for a constant coefficient case by using Fourier analysis (Peaceman, 1980; Douglas & Gunn, 1963,1964). Yauenko, Samarskii and Marchuk study this method (Yanenko, 1967; Marchuk,1990), and Yuan gives a characteristic fractional step difference for a two-dimensional problem and present convergence analysis (Yuan,1999,2003). From the previous work, the authors propose a mixed volume element modified with the characteristic fractional step differnece for a three-dimensional compressible multicomponent displacement problem. The flow equation is treated by a conservative mixed volume element, and the accuracy of Darcy velocity is improved one order. The concentration vector is computed by a second characteristic fractional step difference scheme. Since the method of characteristics is used, numerical dispersion, oscillations and the computational complexity are overcome. A large time step could be adopted without any loss of accuracy. The whole computation is accomplished by solving three successive one-dimensional problems in parallel. A speedup method is used, and the computation is decreased greatly. By the variation, energy norm analysis, the usage of different meshes, piecewise product threefold quadratic interpolation (27-point interpolation) (Ciarlet,1978), decomposition of high-order difference operators and the interchangeability of different operators, we obtain an optimal error estimates in L^2-norm. This work maybe gives some valuable references in the research on numerical simulation of modern oil recovery such as model analysis, numerical method, mechanism study and engineering software (Douglas, 1983b; Ewing,1983; Yuan,2013; Shen, Liu & Tang, 2002).

For convenience, we assume that the problem of (1)-(4) is Ω-periodic. In fact, the boundary condition affects the interior flow slightly (Russell, 1985; Ewing, Russell & Wheeler, 1984; Douglas & Yuan, 1986), thus the boundary condition could be ignored (3). Assume that (1)-(4) is suitably smooth, and the coefficients are positive definite,

$$\text{(C)} \qquad \begin{array}{ll} 0 < \phi_* \le \phi(X) \le \phi^*, & 0 < a_* \le a(c) \le a^*, \\ 0 < d_* \le d(c) \le d^*, & 0 < D_* \le D(X) \le D^*. \end{array}$$

where ϕ_*, ϕ^*, a_*, a^*, d_*, d^*, D_* and D^* are positive constants.

The problem of (1)-(4) is regular,

$$(\mathrm{R}) \qquad \begin{cases} p \in L^\infty(J; H^3(\Omega)) \bigcap H^1(J; W^{4,\infty}(\Omega)), & \frac{\partial p}{\partial t^2} \in L^\infty(L^\infty), \\ c_\alpha \in L^\infty(J; W^{4,\infty}(\Omega)), & \frac{\partial^c_\alpha}{\partial \tau_\alpha^2} \in L^\infty(L^\infty(\Omega)), \alpha = 1, 2, \cdots, n_c - 1. \end{cases}$$

In this paper, the symbols M and ε denote a generic positive constant and a generic small positive number, respectively. They may have different definitions at different places.

2. Notation and Preliminaries

Two different partitions are introduced to formulate the scheme. For simplicity, take $\Omega = [0, 1]^3$. Define the first partition for the flow equation,

$$\begin{aligned} \delta_x &: \ 0 = x_{1/2} < x_{3/2} < \cdots < x_{N_x-1/2} < x_{N_x+1/2} = 1, \\ \delta_y &: \ 0 = y_{1/2} < y_{3/2} < \cdots < y_{N_y-1/2} < y_{N_y+1/2} = 1, \\ \delta_z &: \ 0 = z_{1/2} < z_{3/2} < \cdots < z_{N_z-1/2} < z_{N_z+1/2} = 1. \end{aligned}$$

Ω is partitioned by $\delta_x \times \delta_y \times \delta_z$. For $i = 1, 2, \cdots, N_x$, let $I_i^x = (x_{i-1/2}, x_{i+1/2})$, $x_i = (x_{i-1/2} + x_{i+1/2})/2$, $h_{x_i} = x_{i+1/2} - x_{i-1/2}$, $h_{x,i+1/2} = (h_{x_i} + h_{x_{i+1}})/2 = x_{i+1} - x_i$, $h_x = \max\limits_{1 \le i \le N_x} \{h_{x_i}\}$. I_j^y, I_k^z, y_j, z_k, h_{y_j}, h_{z_k}, $h_{y,j+1/2}$, $h_{z,k+1/2}$, h_y and h_z can be defined similarly for $j = 1, 2, \cdots, N_y$ and $k = 1, 2, \cdots, N_z$. Let $\Omega_{ijk} = I_i^x \times I_j^y \times I_k^z$ and $h_p = (h_x^2 + h_y^2 + h_z^2)^{1/2}$. Suppose that the partition is regular (see Fig. 1 as an example illustration).

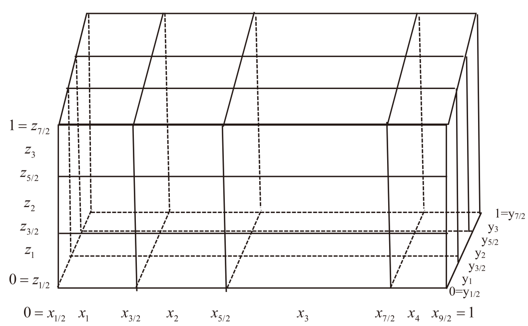

Figure 1. Nonuniform partition

Let $p_d(I_i^x)$ denotes a space where each element is a polynomial function of degree no greater than d constricted on I_i^x, then define an experimental space by $M_l^d(\delta_x) = \{f \in C^l[0, 1] : f|_{I_i^x} \in p_d(I_i^x), i = 1, 2, \cdots, N_x\}$. $f(x)$ may be discontinuous on $[0, 1]$ if $l = -1$. $M_l^d(\delta_y)$ and $M_l^d(\delta_z)$ are defined similarly. Let $S_h = M_{-1}^0(\delta_x) \bigotimes M_{-1}^0(\delta_y) \bigotimes M_{-1}^0(\delta_z)$, $V_h = \{\mathbf{w} | \mathbf{w} = (w^x, w^y, w^z), w^x \in M_0^1(\delta_x) \bigotimes M_{-1}^0(\delta_y) \bigotimes M_{-1}^0(\delta_z), w^y \in M_{-1}^0(\delta_x) \bigotimes M_0^1(\delta_y) \bigotimes M_{-1}^0(\delta_z), w^z \in M_{-1}^0(\delta_x) \bigotimes M_{-1}^0(\delta_y) \bigotimes M_0^1(\delta_z), \mathbf{w} \cdot \gamma|_{\partial\Omega} = 0\}$.

The inner products and norms are defined by

$$(v, w)_m = \sum_{i=1}^{N_x} \sum_{j=1}^{N_y} \sum_{k=1}^{N_z} h_{x_i} h_{y_j} h_{z_k} v_{ijk} w_{ijk}, \ (v, w)_x = \sum_{i=1}^{N_x} \sum_{j=1}^{N_y} \sum_{k=1}^{N_z} h_{x_{i-1/2}} h_{y_j} h_{z_k} v_{i-1/2,jk} w_{i-1/2,jk},$$

$$\|v\|_\infty = \max_{1 \le i \le N_x, 1 \le j \le N_y, 1 \le k \le N_z} |v_{ijk}|, \quad \|v\|_{\infty(x)} = \max_{1 \le i \le N_x, 1 \le j \le N_y, 1 \le k \le N_z} |v_{i-1/2,jk}|,$$

and define $(v, w)_y$, $(v, w)_z$, $\|v\|_{\infty(y)}$, $\|v\|_{\infty(z)}$ similarly. Let $\|v\|_s^2 = (v, v)_s$, $s = m, x, y, z$. For a vector $\mathbf{w} = (w^x, w^y, w^z)^T$, define

$$|||\mathbf{w}||| = \left(\|w^x\|_x^2 + \|w^y\|_y^2 + \|w^z\|_z^2\right)^{1/2}, \ |||\mathbf{w}|||_\infty = \|w^x\|_{\infty(x)} + \|w^y\|_{\infty(y)} + \|w^z\|_{\infty(z)},$$

$$\|\mathbf{w}\|_m = \left(\|w^x\|_m^2 + \|w^y\|_m^2 + \|w^z\|_m^2\right)^{1/2}, \ \|\mathbf{w}\|_\infty = \|w^x\|_\infty + \|w^y\|_\infty + \|w^z\|_\infty.$$

Let $W_p^m(\Omega) = \{v \in L^p(\Omega) | \frac{\partial^n v}{\partial x^{n-l-r} \partial y^l \partial z^r} \in L^p(\Omega), n - l - r \ge 0, l = 0, 1, \cdots, n; r = 0, 1, \cdots, n, n = 0, 1, \cdots, m; 0 \le p \le \infty\}$ and $H^m(\Omega) = W_2^m(\Omega)$. Let $(\cdot, \cdot)$ and $\|\cdot\|$ denote the inner product and norm in $L^2(\Omega)$, respectively. For $\forall v \in S_h$, we have

$$\|v\|_m = \|v\|. \tag{5}$$

The differences are defined by

$$[d_x v]_{i+1/2,jk} = \frac{v_{i+1,jk} - v_{ijk}}{h_{x,i+1/2}}, \qquad [D_x w]_{ijk} = \frac{w_{i+1/2,jk} - w_{i-1/2,jk}}{h_{x_i}},$$
$$\hat{w}^x_{ijk} = \frac{w^x_{i+1/2,jk} + w^x_{i-1/2,jk}}{2}, \qquad \bar{w}^x_{ijk} = \frac{h_{x,i+1}}{2h_{x,i+1/2}} w_{ijk} + \frac{h_{x,i}}{2h_{x,i+1/2}} w_{i+1,jk},$$

and $[d_z v]_{ij,k+1/2}$, $\left[d_y v\right]_{i,j+1/2,k}$, $\left[D_y w\right]_{ijk}$, $[D_z w]_{ijk}$, $\hat{w}^y_{ijk}$, $\hat{w}^z_{ijk}$, $\bar{w}^y_{ijk}$ and $\bar{w}^z_{ijk}$ are defined similarly. Let $\hat{\mathbf{w}}_{ijk} = (\hat{w}^x_{ijk}, \hat{w}^y_{ijk}, \hat{w}^z_{ijk})^T$ and $\bar{\mathbf{w}}_{ijk} = (\bar{w}^x_{ijk}, \bar{w}^y_{ijk}, \bar{w}^z_{ijk})^T$. Let L denote a positive integer, $\Delta t = T/L$, $t^n = n\Delta t$, and $d_t v^n = (v^n - v^{n-1})/\Delta t$.

Several preliminaries are prepared for the following theoretical analysis.

Lemma 1 *For $v \in S_h$ and $\mathbf{w} \in V_h$,*

$$(v, D_x w^x)_m = -(d_x v, w^x)_x, \ \left(v, D_y w^y\right)_m = -\left(d_y v, w^y\right)_y, \ (v, D_z w^z)_m = -(d_z v, w^z)_z. \tag{6}$$

Lemma 2 *For $\mathbf{w} \in V_h$,*

$$\|\hat{\mathbf{w}}\|_m \le |||\mathbf{w}|||. \tag{7}$$

Proof. It requires to prove that $\|\hat{w}^x\|_m \le \|w^x\|_x$, $\|\hat{w}^y\|_m \le \|w^y\|_y$ and $\|\hat{w}^z\|_m \le \|w^z\|_z$. From the fact that

$$\begin{aligned}
\sum_{i=1}^{N_x}\sum_{j=1}^{N_y}\sum_{k=1}^{N_z} h_{x_i} h_{y_j} h_{z_k} (\hat{w}^x_{ijk})^2 &\le \sum_{j=1}^{N_y}\sum_{k=1}^{N_z} h_{y_j} h_{z_k} \sum_{i=1}^{N_x} \frac{(w^x_{i+1/2,jk})^2 + (w^x_{i-1/2,jk})^2}{2} h_{x_i} \\
&= \sum_{j=1}^{N_y}\sum_{k=1}^{N_z} h_{y_j} h_{z_k} \Big(\sum_{i=2}^{N_x} \frac{h_{x,i-1}}{2} (w^x_{i-1/2,jk})^2 + \sum_{i=1}^{N_x} \frac{h_{x_i}}{2} (w^x_{i-1/2,jk})^2 \Big) \\
&= \sum_{j=1}^{N_y}\sum_{k=1}^{N_z} h_{y_j} h_{z_k} \sum_{i=2}^{N_x} \frac{h_{x,i-1} + h_{x_i}}{2} (w^x_{i-1/2,jk})^2 \\
&= \sum_{i=1}^{N_x}\sum_{j=1}^{N_y}\sum_{k=1}^{N_z} h_{x,i-1/2} h_{y_j} h_{z_k} (w^x_{i-1/2,jk})^2,
\end{aligned}$$

we have $\|\hat{w}^x\|_m \le \|w^x\|_x$. Similarly, other inequalities are proved.

Lemma 3 *For $q \in S_h$, For $q \in S_h$, there exists a number M independent of q, h such that*

$$\|\bar{q}^x\|_x \le M\|q\|_m, \ \|\bar{q}^y\|_y \le M\|q\|_m, \ \|\bar{q}^z\|_z \le M\|q\|_m. \tag{8}$$

Lemma 4 *For $\mathbf{w} \in V_h$,*

$$\|w^x\|_x \le \|D_x w^x\|_m, \ \|w^y\|_y \le \|D_y w^y\|_m, \ \|w^z\|_z \le \|D_z w^z\|_m. \tag{9}$$

Proof. $\|w^x\|_x \le \|D_x w^x\|_{\bar{m}}$ is proved first. Note that

$$w^x_{l+1/2,jk} = \sum_{i=1}^{l} (w^x_{i+1/2,jk} - w^x_{i-1/2,jk}) = \sum_{i=1}^{l} \frac{w^x_{i+1/2,jk} - w^x_{i-1/2,jk}}{h_{x_i}} h^{1/2}_{x_i} h^{1/2}_{x_i},$$

and use the Cauchy inequality, we have

$$(w^x_{l+1/2,jk})^2 \le x_l \sum_{i=1}^{N_x} h_{x_i} (\, [D_x w^x]_{ijk}\,)^2.$$

Multiply the both sides by $h_{x,i+1/2} h_{y_j} h_{z_k}$, and make the sum,

$$\sum_{i=1}^{N_x}\sum_{j=1}^{N_y}\sum_{k=1}^{N_z} (w^x_{i-1/2,jk})^2 h_{x,i-1/2} h_{y_j} h_{z_k} \le \sum_{i=1}^{N_x}\sum_{j=1}^{N_y}\sum_{k=1}^{N_z} (\, [D_x w^x]_{ijk}\,)^2 h_{x_i} h_{y_j} h_{z_k}.$$

The proof ends.

Another refined partition of $\Omega = \{[0,1]\}^3$ is defined by $\bar{\delta}_x \times \bar{\delta}_y \times \bar{\delta}_z$,

$$\begin{aligned}
\bar{\delta}_x &: \ 0 = x_0 < x_1 < \cdots < x_{M_1-1} < x_{M_1} = 1,\\
\bar{\delta}_y &: \ 0 = y_0 < y_1 < \cdots < y_{M_2-1} < y_{M_2} = 1,\\
\bar{\delta}_z &: \ 0 = z_0 < z_1 < \cdots < z_{M_3-1} < z_{M_3} = 1.
\end{aligned}$$

Here M_1, M_2 and M_3 are positive constants. Let $h^x = \frac{1}{M_1}$, $h^y = \frac{1}{M_2}$, $h^z = \frac{1}{M_3}$, $x_i = i \cdot h^x$, $y_j = j \cdot h^y$, $z_k = k \cdot h^z$, $h = ((h^x)^2 + (h^y)^2 + (h^z)^2)^{1/2}$. Define $D_{i+1/2,jk} = \frac{1}{2}[D(X_{ijk}) + D(X_{i+1,jk})]$, $D_{i-1/2,jk} = \frac{1}{2}[D(X_{ijk}) + D(X_{i-1,jk})]$. $D_{i,j+1/2,k}$, $D_{i,j-1/2,k}$, $D_{ij,k+1/2}$ and $D_{ij,k-1/2}$ are given similarly. Let

$$\delta_{\bar{x}}(D\delta_x W)^n_{ijk} = (h^x)^{-2}[D_{i+1/2,jk}(W^n_{i+1,jk} - W^n_{ijk}) - D_{i-1/2,jk}(W^n_{ijk} - W^n_{i-1,jk})], \tag{10a}$$

$$\delta_{\bar{y}}(D\delta_y W)^n_{ijk} = (h^y)^{-2}[D_{i,j+1/2,k}(W^n_{i,j+1,k} - W^n_{ijk}) - D_{i,j-1/2,k}(W^n_{ijk} - W^n_{i,j-1,k})], \tag{10b}$$

$$\delta_{\bar{z}}(D\delta_z W)^n_{ijk} = (h^z)^{-2}[D_{ij,k+1/2}(W^n_{ij,k+1} - W^n_{ijk}) - D_{ij,k-1/2}(W^n_{ijk} - W^n_{ij,k-1})]. \tag{10c}$$

$$\nabla_h(D\nabla W)^n_{ijk} = \delta_{\bar{x}}(D\delta_x W)^n_{ijk} + \delta_{\bar{y}}(D\delta_y W)^n_{ijk} + \delta_{\bar{z}}(D\delta_z W)^n_{ijk}. \tag{11}$$

3. The Procedures

The flow equation (1) is rewritten in a normal form to construct the mixed volume element,

$$d(c)\frac{\partial p}{\partial t} + \nabla \cdot \mathbf{u} = q(X,t), \ (X,t) \in \Omega \times J, \tag{12a}$$

$$\mathbf{u} = -a(c)\nabla p, \ (X,t) \in \Omega \times J. \tag{12b}$$

Let P, $\mathbf{U}$ and C denote the numerical solutions of p, $\mathbf{u}$ and c, respectively. Here C is computed by a threefold quadratic interpolation on the refined partition Ω_h (Yuan, 2013; Ciarlet, 1978). Recalling the notation and preliminary properties, we obtain the mixed volume element procedures for the pressure and Darcy velocity (Russell, 1995; Weiser & Wheeler, 1988; Jones, 1995),

$$\left(d(C^n)\frac{P^{n+1} - P^n}{\Delta t}, v\right)_m + \left(D_x U^{x,n+1} + D_y U^{y,n+1} + D_z U^{z,n+1}, v\right)_m = \left(q^{n+1}, v\right)_m, \ \forall\, v \in S_h, \tag{13a}$$

$$\begin{aligned}
&\left(a^{-1}(\bar{C}^{x,n})U^{x,n+1}, w^x\right)_x + \left(a^{-1}(\bar{C}^{y,n})U^{y,n+1}, w^y\right)_y + \left(a^{-1}(\bar{C}^{z,n})U^{z,n+1}, w^z\right)_z\\
&- \left(P^{n+1}, D_x w^x + D_x w^y + D_z w^z\right)_m = 0, \forall\, \mathbf{w} \in V_h.
\end{aligned} \tag{13b}$$

The flow shown in Eq. (2) moves along the characteristics, so the method of characteristics is used to approximate the hyperbolic term. This treatment has strong stability and high accuracy. A large time step may be used during the computations. Let $\psi(X,\mathbf{u}) = [\phi^2(X) + |\mathbf{u}|^2]^{1/2}$ and $\frac{\partial}{\partial \tau} = \psi^{-1}\{\phi\frac{\partial}{\partial t} + \mathbf{u}\cdot\nabla\}$. A backward difference quotient is given for the derivative along the characteristic direction,

$$\frac{\partial c^{n+1}_\alpha}{\partial \tau}(X) \approx \frac{c^{n+1}_\alpha - c^n_\alpha(X - \phi^{-1}\mathbf{u}^{n+1}(X)\Delta t)}{\Delta t(1 + \phi^{-2}|\mathbf{u}^{n+1}|^2)^{1/2}}.$$

Then, the characteristic fractional step difference scheme is concluded for Eq. (2),

$$\begin{aligned}
\phi_{ijk}\frac{C^{n+1/3}_{\alpha,ijk} - \hat{C}^n_{\alpha,ijk}}{\Delta t} &= \delta_{\bar{x}}(D\delta_x C^{n+1/3}_\alpha)_{ijk} + \delta_{\bar{y}}(D\delta_y C^n_\alpha)_{ijk} + \delta_{\bar{z}}(D\delta_z C^n_\alpha)_{ijk}\\
&\quad - b_\alpha(C^n_{ijk})\frac{P^{n+1}_{ijk} - P^n_{ijk}}{\Delta t} + g(X_{ijk}, t^n, \hat{C}^n_{\alpha,ijk}), \ 1 \le i \le M_1, \alpha = 1,2,\cdots,n_c - 1,
\end{aligned} \tag{14}$$

$$\phi_{ijk}\frac{C^{n+2/3}_{\alpha,ijk} - C^{n+1/3}_{\alpha,ijk}}{\Delta t} = \delta_{\bar{y}}(D\delta_y(C^{n+2/3}_\alpha - C^n_\alpha))_{ijk}, \ 1 \le j \le M_2, \alpha = 1,2,\cdots,n_c - 1, \tag{15}$$

$$\phi_{ijk}\frac{C^{n+1}_{\alpha,ijk} - C^{n+2/3}_{\alpha,ijk}}{\Delta t} = \delta_{\bar{z}}(D\delta_z(C^{n+1}_\alpha - C^n_\alpha))_{ijk}, \ 1 \le k \le M_3, \alpha = 1,2,\cdots,n_c - 1, \tag{16}$$

where $C^n_\alpha(X)(\alpha = 1,2,\cdots,n_c - 1)$ is determined by a threefold quadratic interpolation of $\{C^n_{\alpha,ijk}\}$ at twenty-seven points nearby, $\hat{C}^n_{\alpha,ijk} = C^n_\alpha(\hat{X}^n_{ijk})$, $\hat{X}^n_{ijk} = X_{ijk} - \phi^{-1}_{ijk}\mathbf{U}^{n+1}_{ijk}\Delta t$.

Initial approximations,

$$P^0_{ijk} = p_0(X_{ijk}),\ C^0_{\alpha,ijk} = c_{\alpha,0}(X_{ijk}),\ X_{ijk} \in \bar{\Omega}_h,\ \alpha = 1, 2, \cdots, n_c - 1. \tag{17}$$

The composite procedures run as follows. From (17) and the elliptic projections $\{\tilde{\mathbf{U}}^0, \tilde{P}^0\}$ (seen in the next section), take $\mathbf{U}^0 = \tilde{\mathbf{U}}^0$ and $P^0 = \tilde{P}^0$. Using the scheme (13) and the method of conjugate gradient, we get $\{\mathbf{U}^1, P^1\}$. Then, from (14)-(16) and the speedup algorithm, $\{C^1_\alpha\}, \alpha = 1, 2, \cdots, n_c - 1\}$ is computed in parallel. Repeat the computations as above, we could all the numerical solutions. From (C), we find that the solutions exist and are unique.

4. Convergence Analysis

Introduce the elliptic projections first. Define $\tilde{\mathbf{U}} \in V_h$, $\tilde{P} \in S_h$,

$$\left(D_x\tilde{U}^x + D_y\tilde{U}^y + D_z\tilde{U}^z, v\right)_m = (\nabla\cdot\mathbf{u}, v)_m\,, \forall\ v \in S_h, \tag{18a}$$

$$\left(a^{-1}(c)\tilde{U}^x, w^x\right)_x + \left(a^{-1}(c)\tilde{U}^y, w^y\right)_y + \left(a^{-1}(c)\tilde{U}^z, w^z\right)_z - \left(\tilde{P}, D_xw^x + D_yw^y + D_zw^z\right)_m = 0, \forall\ \mathbf{w} \in V_h, \tag{18b}$$

$$\left(\tilde{P} - p, 1\right)_m = 0. \tag{18c}$$

Let $\pi = P - \tilde{P}$, $\eta = \tilde{P} - p$, $\sigma = \mathbf{U} - \tilde{\mathbf{U}}$, $\rho = \tilde{\mathbf{U}} - \mathbf{u}$, $\xi = c - C$. Suppose that the problem of (1) and (2) is positive definite (C) and properly regular (R). From the theory of Weiser and Wheeler (Weiser & Wheeler, 1988; Jones, 1995), it is easy to see that the solutions of (18), $\tilde{\mathbf{U}}$ and $\tilde{P}$ exist and are estimated in Lemma 5.

Lemma 5 *Under the conditions (C) and (R), there exist two positive constants $\bar{C}_1$ and $\bar{C}_2$ independent of $h, \Delta t$ such that*

$$\|\eta\|_m + |||\rho||| \le \bar{C}_1 h_p^2, \tag{19a}$$

$$\left\|\frac{\partial\eta}{\partial t}\right\|_\infty + \left|\left|\left|\tilde{\mathbf{U}}\right|\right|\right|_\infty + \left|\left|\left|\frac{\partial\tilde{\mathbf{U}}}{\partial t}\right|\right|\right|_\infty \le \bar{C}_2. \tag{19b}$$

Discuss π and σ first. Subtracting (18a) ($t = t^{n+1}$) and (18b) ($t = t^{n+1}$) from (13a) and (13b), respectively,

$$\begin{aligned}
&(d(C^n)\partial_t\pi^n, v)_m + \left(D_x\sigma^{x,n+1} + D_y\sigma^{y,n+1} + D_z\sigma^{z,n+1}, v\right)_m \\
&= \left((d(c^{n+1}) - d(C^n))\frac{\partial\tilde{p}^{n+1}}{\partial t}, v\right)_m - \left(d(c^{n+1})\partial_t\eta^n, v\right)_m + \left(d(C^n)(\frac{\partial\tilde{p}^{n+1}}{\partial t} - \partial_t\tilde{P}^n), v\right)_m, \forall\ v \in S_h,
\end{aligned} \tag{20a}$$

$$\begin{aligned}
&\left(a^{-1}(\bar{C}^{x,n})\sigma^{x,n+1}, w^x\right)_x + \left(a^{-1}(\bar{C}^{y,n})\sigma^{y,n+1}, w^y\right)_y + \left(a^{-1}(\bar{C}^{z,n})\sigma^{z,n+1}, w^z\right)_z \\
&- \left(\pi^{n+1}, D_xw^x + D_yw^y + D_zw^z\right)_m \\
&= -\left((a^{-1}(\bar{C}^{x,n}) - a^{-1}(c^{n+1}))\tilde{U}^{x,n+1}, w^x\right)_x - \left((a^{-1}(\bar{C}^{y,n}) - a^{-1}(c^{n+1}))\tilde{U}^{y,n+1}, w^y\right)_y \\
&- \left((a^{-1}(\bar{C}^{z,n}) - a^{-1}(c^{n+1}))\tilde{U}^{z,n+1}, w^z\right)_z,\ \forall\ \mathbf{w} \in V_h,
\end{aligned} \tag{20b}$$

where $\partial_t\pi^n = (\pi^{n+1} - \pi^n)/\Delta t$.

Take $v = \partial_t\pi^n$ in (20a). Divide the difference of (20b) at t^{n+1} and t^n by Δt, and take $\mathbf{w} = \sigma^{n+1}$. For $A^n \ge 0$, we have

$$\begin{aligned}
\left(\partial_t(A^{n-1}B^n), B^{n+1}\right)_s &= \frac{1}{2}\partial_t\left(A^{n-1}B^n, B^n\right)_s - \frac{1}{2}\left(\partial_t(A^{n-1})B^n, B^n\right)_s + \left(\partial_t(A^{n-1})B^n, B^{n+1}\right)_s \\
&+ \frac{1}{2\Delta t}\left(A^n(B^{n+1} - B^n), B^{n+1} - B^n\right)_s \\
&\ge \frac{1}{2}\partial_t\left(AB^n, B^n\right)_s - \frac{1}{2}\left(\partial_t(A^{n-1})B^n, B^n\right)_s + \left(\partial_t(A^{n-1})B^n, B^{n+1}\right)_s,\ s = x, y, z.
\end{aligned}$$

Thus,

$$\begin{aligned}
&d_*\|\partial_t\pi^n\|_m^2 + \frac{1}{2}\partial_t\left[\left(a^{-1}(\bar{C}^{x,n})\sigma^{x,n}, \sigma^{x,n}\right)_x + \left(a^{-1}(\bar{C}^{y,n})\sigma^{y,n}, \sigma^{y,n}\right)_y + \left(a^{-1}(\bar{C}^{z,n})\sigma^{z,n}, \sigma^{z,n}\right)_z\right] \\
&\le \left((d(c^{n+1}) - d(C^n))\frac{\partial\tilde{p}^{n+1}}{\partial t}, \partial_t\pi^n\right)_m - \left(d(c^{n+1})\frac{\partial\eta^{n+1}}{\partial t}, \partial_t\pi^n\right)_m + \left(d(C^n)(\frac{\partial\tilde{p}^{n+1}}{\partial t} - \partial_t\tilde{P}^n), \partial_t\pi^n\right)_m \\
&- \left\{\left(\partial_t[(a^{-1}(\bar{C}^{x,n-1}) - a^{-1}(c^{n-1}))\tilde{\mathbf{U}}^{x,n}], \sigma^{x,n+1}\right)_x + \left(\partial_t[(a^{-1}(\bar{C}^{y,n-1}) - a^{-1}(c^{n-1}))\tilde{\mathbf{U}}^{y,n}], \sigma^{y,n+1}\right)_y\right.
\end{aligned}$$

$$
\begin{aligned}
&+\left(\partial_t[(a^{-1}(\bar{C}^{z,n-1})-a^{-1}(c^{n-1}))\tilde{\mathbf{U}}^{z,n}],\sigma^{z,n+1}\right)_z\Big\}-\Big\{\left(\partial_t[(a^{-1}(c^n)-a^{-1}(c^{n-1}))\tilde{\mathbf{U}}^{x,n}],\sigma^{x,n+1}\right)_x\\
&+\left(\partial_t[(a^{-1}(c^n)-a^{-1}(c^{n-1}))\tilde{\mathbf{U}}^{y,n}],\sigma^{y,n+1}\right)_y+\left(\partial_t[(a^{-1}(c^n)-a^{-1}(c^{n-1}))\tilde{\mathbf{U}}^{z,n}],\sigma^{z,n+1}\right)_z\Big\}\\
&+\frac{1}{2}\Big\{\partial_t(a^{-1}(\bar{C}^{x,n-1})\sigma^{x,n},\sigma^{x,n})_x+\partial_t(a^{-1}(\bar{C}^{y,n-1})\sigma^{y,n},\sigma^{y,n})_y \qquad (21)\\
&+\partial_t(a^{-1}(\bar{C}^{z,n-1})\sigma^{z,n},\sigma^{z,n})_z\Big\}-\frac{1}{2}\Big\{\left(\partial_t(a^{-1}(\bar{C}^{x,n-1}))\sigma^{x,n},\sigma^{x,n+1}\right)_x\\
&+\left(\partial_t(a^{-1}(\bar{C}^{y,n-1}))\sigma^{y,n},\sigma^{y,n+1}\right)_y+\left(\partial_t(a^{-1}(\bar{C}^{z,n-1}))\sigma^{z,n},\sigma^{z,n+1}\right)_z\Big\}=T_1+T_2+\cdots+T_7.
\end{aligned}
$$

From Lemma 5,

$$|T_1+T_2+T_3|\le\varepsilon\left\|\partial_t\pi^n\right\|_m^2+M\{\left\|\xi^n\right\|_m^2+h_p^4+(\Delta t)^2\}. \tag{22}$$

Introduce an induction hypothesis,

$$\sup_{0\le n\le L}\left|\left|\left|\sigma\right|\right|\right|_\infty\to 0,\ \sup_{0\le n\le L}\left\|\xi^n\right\|_\infty\to 0,\quad (h,h_p,\Delta t)\to 0. \tag{23}$$

Using the fact that $\partial_t(a^{-1}(\bar{C}^{x,n-1}))=\frac{da^{-1}}{dc}\partial_t(\bar{C}^{x,n-1})=\frac{da^{-1}}{dc}[\partial_t(c^{x,n-1})+\partial_t(\xi^{x,n-1})]$, and Lemma 4, Lemma 5, we have

$$|T_5|\le M\{(\Delta t)^2+\left|\left|\left|\sigma^{n+1}\right|\right|\right|^2\}, \tag{24a}$$

$$
\begin{aligned}
|T_6+T_7|&\le M\{\left|\left|\left|\sigma^n\right|\right|\right|^2+\left|\left|\left|\sigma^n\right|\right|\right|\cdot\left|\left|\left|\sigma^{n+1}\right|\right|\right|+\left|\left|\left|\sigma\right|\right|\right|_\infty\left\|\partial_t\xi^{n-1}\right\|_m(\left|\left|\left|\sigma^n\right|\right|\right|+\left|\left|\left|\sigma^{n+1}\right|\right|\right|)\}\\
&\le\varepsilon\left\|\partial_t\xi^{n-1}\right\|_m^2+M\{\left|\left|\left|\sigma^n\right|\right|\right|^2+\left|\left|\left|\sigma^{n+1}\right|\right|\right|^2\}.
\end{aligned}\tag{24b}
$$

T_4 is estimated by using (R), the Taylor expansion, Lemma 5 and (23),

$$|T_4|\le\varepsilon\left\|\partial_t\xi^{n-1}\right\|_m^2+M\{\left\|\xi^n\right\|_m^2+\left\|\xi^{n-1}\right\|_m^2+\left|\left|\left|\sigma^{n+1}\right|\right|\right|^2+h_p^4+(\Delta t)^2\}. \tag{24c}$$

Substituting (22) and (24) into (21) to find

$$
\begin{aligned}
&\|\partial_t\pi^n\|_m^2+\partial_t\sum_{s=x,y,z}\left(a^{-1}(\bar{C}^{s,n})\sigma^{s,n},\sigma^{s,n}\right)_s\\
&\le\varepsilon\left\|\partial_t\xi^{n-1}\right\|_m^2+M\{\left\|\xi^n\right\|_m^2+\left\|\xi^{n-1}\right\|_m^2+\left|\left|\left|\sigma^n\right|\right|\right|^2+\left|\left|\left|\sigma^{n+1}\right|\right|\right|^2+h_p^4+(\Delta t)^2\}.
\end{aligned}\tag{25}
$$

Taking $v=\pi^{n+1}$ in (20a) and $\mathbf{w}=\sigma^{n+1}$ in (20b), and making the sum, we have

$$
\begin{aligned}
(d(C^n)\partial_t\pi^n,\pi^n)_m&=\frac{1}{2}\partial_t(d(C^n)\pi^n,\pi^n)_m-\frac{1}{2}(\partial_t(d(C^n))\pi^n,\pi^n)_m\\
&\quad+\frac{1}{2\Delta t}((d(C^n))(\pi^{n+1}-\pi^n),\pi^{n+1}-\pi^n)_m\\
&\ge\frac{1}{2}\partial_t(d(C^n)\pi^n,\pi^n)_m-\frac{1}{2}(\partial_t(d(C^n))\pi^n,\pi^n)_m.
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
&\frac{1}{2}\partial_t(d(C^n)\pi^n,\pi^n)_m-\frac{1}{2}(\partial_t(d(C^n))\pi^n,\pi^n)_m+\left(a^{-1}(\bar{C}^{x,n})\sigma^{x,n+1},\sigma^{x,n+1}\right)_x\\
&+\left(a^{-1}(\bar{C}^{y,n})\sigma^{y,n+1},\sigma^{y,n+1}\right)_y+\left(a^{-1}(\bar{C}^{z,n})\sigma^{z,n+1},\sigma^{z,n+1}\right)_z\\
&\le\left((d(c^{n+1})-d(C^n))\frac{\partial\tilde{p}^{n+1}}{\partial t},\pi^{n+1}\right)_m-\left(d(c^{n+1})\partial_t\eta^n,\pi^{n+1}\right)_m+\left(d(C^n)(\frac{\partial\tilde{p}^{n+1}}{\partial t}-\partial_t\tilde{P}^n),\pi^{n+1}\right)_m\\
&-\sum_{s=x,y,z}\left((a^{-1}(\bar{C}^{s,n})-a^{-1}(c^{n+1}))\tilde{U}^{s,n+1},\sigma^{s,n+1}\right)_s.
\end{aligned}\tag{26}
$$

Let $d'_c=d'(c)$, and we have

$$
\begin{aligned}
\left|(\partial_t(d(C^n))\pi^n,\pi^n)_m\right|&=\left|(d'_c(\partial_t(c^{n-1})+\partial_t\xi^{n-1})\pi^n,\pi^n)_m\right|\\
&\le\varepsilon\left\|\partial_t\xi^{n-1}\right\|_m^2+M\left\|\pi^n\right\|_m^2.
\end{aligned}\tag{27}
$$

Then, it follows (26),

$$\partial_t(d(C^n)\pi^n,\pi^n)_m + \left|\left|\left|\sigma^{n+1}\right|\right|\right|^2 \le \varepsilon\left\|\partial_t\xi^{n-1}\right\|_m^2 + M\{\left\|\pi^n\right\|_m^2 + \left\|\pi^{n+1}\right\|_m^2 + h_p^4 + (\Delta t)^2\}, \tag{28}$$

Combining (25) and (28) to see that

$$\begin{aligned}&\|\partial_t\pi^n\|_m^2 + \partial_t\sum_{s=x,y,z}\left(a^{-1}(\bar{C}^{s,n})\sigma^{s,n},\sigma^{s,n}\right)_s + \partial_t(d(C^n)\pi^n,\pi^n)_m + \left|\left|\left|\sigma^{n+1}\right|\right|\right|^2\\ &\le \varepsilon\left\|\partial_t\xi^{n-1}\right\|_m^2 + M\{\left\|\pi^n\right\|_m^2 + \left\|\pi^{n+1}\right\|_m^2 + \left\|\xi^n\right\|_m^2 + \left\|\xi^{n-1}\right\|_m^2 + \left|\left|\left|\sigma^n\right|\right|\right|^2 + \left|\left|\left|\sigma^{n+1}\right|\right|\right|^2 + h_p^4 + (\Delta t)^2\},\end{aligned} \tag{29}$$

The partition of $\Omega = \{[0,1]\}^3$ is denoted by $\bar{\Omega}_h = \Omega_h \cup \partial\Omega_h = \bar{\omega}_1\times\bar{\omega}_2\times\bar{\omega}_3$ consisting of rectangular solids, where $\bar{\omega}_1 = \{x_i|i = 0,1,\cdots,M_1\}$, $\bar{\omega}_2 = \{y_j|j = 0,1,\cdots,M_2\}$, $\bar{\omega}_3 = \{z_k|k = 0,1,\cdots,M_3\}$, $\omega_1^+ = \{x_i|i = 1,2,\cdots,M_1\}$, $\omega_2^+ = \{y_j|j = 1,2,\cdots,M_2\}$ and $\omega_3^+ = \{z_k|k = 1,2,\cdots,M_3\}$. Let $|f|_0 = \langle f,f\rangle^{1/2}$ denote the norm of discrete space of $L^2(\Omega)$, and

$$\langle f,g\rangle = \sum_{\bar{\omega}_1}h_i^x\sum_{\bar{\omega}_2}h_j^y\sum_{\bar{\omega}_3}h_k^z f(X_{ijk})g(X_{ijk}), \tag{30a}$$

denote the inner product. Here define $h_i^x = h^x, 1\le i\le M_1-1, h_0^x = h_{M_1}^x = h^x/2$; $h_j^y = h^y, 1\le j\le M_2-1, h_0^y = h_{M_2}^y = h^y/2$; $h_k^z = h^z, 1\le k\le M_3-1, h_0^z = h_{M_3}^z = h^z/2$. $\langle D\nabla_h f,\nabla_h f\rangle$ is the square of weighted semi-norm in $h^1(\Omega)$, the discrete space of $H^1(\Omega) = W^{1,2}(\Omega)$ for a positive definite function $D(X)$,

$$\begin{aligned}\langle D\nabla_h f,\nabla_h f\rangle = &\sum_{\bar{\omega}_2}\sum_{\bar{\omega}_3}h_j^y h_k^z\sum_{\omega_1^+}h_i^x\{D(X)[\delta_{\bar{x}}f(X)]^2\} + \sum_{\bar{\omega}_3}\sum_{\bar{\omega}_1}h_k^z h_i^x\sum_{\omega_2^+}h_j^y\{D(X)[\delta_{\bar{y}}f(X)]^2\}\\ &+\sum_{\bar{\omega}_1}\sum_{\bar{\omega}_2}h_i^x h_j^y\sum_{\omega_3^+}h_k^z\{D(X)[\delta_{\bar{z}}f(X)]^2\}.\end{aligned} \tag{30b}$$

The concentration vector is argued later. Eliminating $C_\alpha^{n+1/3}$ and $C_\alpha^{n+2/3}$ from (14)-(16),

$$\begin{aligned}&\phi_{ijk}\frac{C_{\alpha,ijk}^{n+1} - \hat{C}_{\alpha,ijk}^n}{\Delta t} - \sum_{s=x,y,z}\delta_{\bar{s}}(D\delta_s C_\alpha^{n+1})_{ijk}\\ &= -b_\alpha(C_{ijk}^n)\frac{P_{ijk}^{n+1} - P_{ijk}^n}{\Delta t} + g(X_{ijk},t^n,\hat{C}_\alpha^n) - (\Delta t)^2\Big\{\delta_{\bar{x}}(D\delta_x(\phi^{-1}\delta_{\bar{y}}(D\delta_y(\partial_t C_\alpha^n))))_{ijk}\\ &\quad+\delta_{\bar{x}}(D\delta_x(\phi^{-1}\delta_{\bar{z}}(D\delta_z(\partial_t C_\alpha^n))))_{ijk} + \delta_{\bar{y}}(D\delta_y(\phi^{-1}\delta_{\bar{z}}(D\delta_z(\partial_t C_\alpha^n))))_{ijk}\Big\}\\ &\quad+(\Delta t)^3\delta_{\bar{x}}(D\delta_x(\phi^{-1}\delta_{\bar{y}}(D\delta_y(\phi^{-1}\delta_{\bar{z}}(D\delta_z(\partial_t C_\alpha^n))))))_{ijk},\ X_{ijk}\in\Omega_h, \alpha = 1,2,\cdots,n_c-1.\end{aligned} \tag{31}$$

An inequivalent form is derived from (2) ($t = t^{n+1}$) and (31) ($t = t^{n+1}$),

$$\begin{aligned}&\phi_{ijk}\frac{\xi_{\alpha,ijk}^{n+1} - (c_\alpha^n(\bar{X}_{ijk}^n) - \hat{C}_{\alpha,ijk}^n)}{\Delta t} - \sum_{s=x,y,z}\delta_{\bar{s}}(D\delta_s\xi_\alpha^{n+1})_{ijk}\\ &= g(X_{ijk},t^{n+1},c_{\alpha,ijk}^{n+1}) - g(X_{ijk},t^n,\hat{C}_{\alpha,ijk}^n) - b_\alpha(C_{ijk}^n)\frac{\pi_{ijk}^{n+1} - \pi_{ijk}^n}{\Delta t} - [b_\alpha(c_{ijk}^{n+1}) - b_\alpha(C_{ijk}^n)]\frac{p_{ijk}^{n+1} - p_{ijk}^n}{\Delta t}\\ &- (\Delta t)^2\Big\{\delta_{\bar{x}}(D\delta_x(\phi^{-1}\delta_{\bar{y}}(D\delta_y(\partial_t\xi_\alpha^n))))_{ijk} + \delta_{\bar{x}}(D\delta_x(\phi^{-1}\delta_{\bar{z}}(D\delta_z(\partial_t\xi_\alpha^n))))_{ijk}\\ &\quad+\delta_{\bar{y}}(D\delta_y(\phi^{-1}\delta_{\bar{z}}(D\delta_z(\partial_t\xi_\alpha^n))))_{ijk}\Big\}\\ &+(\Delta t)^3\delta_{\bar{x}}(D\delta_x(\phi^{-1}\delta_{\bar{y}}(D\delta_y(\phi^{-1}\delta_{\bar{z}}(D\delta_z(\partial_t\xi_\alpha^n))))))_{ijk} + \varepsilon_{\alpha,ijk}^{n+1},\ X_{ijk}\in\Omega_h, \alpha = 1,2,\cdots,n_c-1,\end{aligned} \tag{32}$$

where $\bar{X}_{ijk}^{n+1} = X_{ijk} - \phi_{ijk}^{-1}\mathbf{u}_{ijk}^{n+1}\Delta t$, $\left|\varepsilon_{\alpha,ijk}^{n+1}\right| \le K\left\{h^2 + \Delta t\right\}$.
Suppose that the partition has the following restriction

$$\Delta t = O(h^2),\quad h^2 = o(h_p^{3/2}). \tag{33}$$

Then, we have

$$\begin{aligned}
&\phi_{ijk}\frac{\xi^{n+1}_{\alpha,ijk}-\hat{\xi}^{n}_{\alpha,ijk}}{\Delta t}-\sum_{s=x,y,z}\delta_{\bar{s}}(D\delta_s\xi^{n+1}_{\alpha})_{ijk}\\
&\le M\Big\{\sum_{\alpha=1}^{n_c-1}\big|\xi^n_{\alpha,ijk}\big|+\big|\mathbf{u}^{n+1}_{ijk}-\mathbf{U}^{n+1}_{ijk}\big|+h^2+\Delta t\Big\}-b_\alpha(C^n_{ijk})\frac{\pi^{n+1}_{ijk}-\pi^n_{ijk}}{\Delta t}\\
&-(\Delta t)^2\Big\{\delta_{\bar{x}}(D\delta_x(\phi^{-1}\delta_{\bar{y}}(D\delta_y(\partial_t\xi^n_\alpha))))_{ijk}+\delta_{\bar{x}}(D\delta_x(\phi^{-1}\delta_{\bar{z}}(D\delta_z(\partial_t\xi^n_\alpha))))_{ijk}\\
&+\delta_{\bar{y}}(D\delta_y(\phi^{-1}\delta_{\bar{z}}(D\delta_z(\partial_t\xi^n_\alpha))))_{ijk}\Big\}+(\Delta t)^3\delta_{\bar{x}}(D\delta_x(\phi^{-1}\delta_{\bar{y}}(D\delta_y(\phi^{-1}\delta_{\bar{z}}(D\delta_z(\partial_t\xi^n_\alpha))))))_{ijk},\ X_{ijk}\in\Omega_h.
\end{aligned}\tag{34}$$

Multiplying both sides of (34) by $\partial_t\xi^n_{\alpha,ijk}\Delta t=\xi^{n+1}_{\alpha,ijk}-\xi^n_{\alpha,ijk}$ and using the summation by parts, we get an inner-product expression,

$$\begin{aligned}
&\Big\langle\phi\frac{\xi^{n+1}_{\alpha}-\hat{\xi}^{n}_{\alpha}}{\Delta t},\partial_t\xi^n_\alpha\Big\rangle\Delta t+\frac{1}{2}\sum_{s=x,y,z}\Big\{\langle D\delta_s\xi^{n+1}_\alpha,\delta_s\xi^{n+1}_\alpha\rangle-\langle D\delta_s\xi^{n}_\alpha,\delta_s\xi^{n}_\alpha\rangle\Big\}\\
&\le\varepsilon\big|\partial_t\xi^n_\alpha\big|_0^2\Delta t+M\Big\{\sum_{\alpha=1}^{n_c-1}\big|\xi^n_\alpha\big|_0^2+|||\sigma^{n+1}|||+h_p^4+h^4+(\Delta t)^2\Big\}\Delta t-\langle b_\alpha(C^n)\partial_t\pi^n,\partial_t\xi^n\rangle\Delta t\\
&-(\Delta t)^3\Big\{\langle\delta_{\bar{x}}(D\delta_x(\phi^{-1}\delta_{\bar{y}}(D\delta_y(\partial_t\xi^n_\alpha)))),\partial_t\xi^n_\alpha\rangle+\langle\delta_{\bar{x}}(D\delta_x(\phi^{-1}\delta_{\bar{z}}(D\delta_z(\partial_t\xi^n_\alpha)))),\partial_t\xi^n_\alpha\rangle\\
&+\langle\delta_{\bar{y}}(D\delta_y(\phi^{-1}\delta_{\bar{z}}(D\delta_z(\partial_t\xi^n_\alpha)))),\partial_t\xi^n_\alpha\rangle\Big\}+(\Delta t)^4\langle\delta_{\bar{x}}(D\delta_x(\phi^{-1}\delta_{\bar{y}}(D\delta_y(\phi^{-1}\delta_{\bar{z}}(D\delta_z(\partial_t\xi^n_\alpha)))))),\partial_t\xi^n_\alpha\rangle.
\end{aligned}\tag{35}$$

The relation of different norms in $L^2(\Omega)$ and $l^2(\Omega)$ is used in the above expression (Yuan, 1992, 19931; Douglas, 1982). From (35),

$$\begin{aligned}
&\Big\langle\phi\frac{\xi^{n+1}_{\alpha}-\xi^{n}_{\alpha}}{\Delta t},\partial_t\xi^n_\alpha\Big\rangle\Delta t+\frac{1}{2}\sum_{s=x,y,z}\Big\{\langle D\delta_s\xi^{n+1}_\alpha,\delta_s\xi^{n+1}_\alpha\rangle-\langle D\delta_s\xi^{n}_\alpha,\delta_s\xi^{n}_\alpha\rangle\Big\}\\
&\le\Big\langle\phi\frac{\hat{\xi}^{n}_{\alpha}-\xi^{n}_{\alpha}}{\Delta t},\partial_t\xi^n_\alpha\Big\rangle\Delta t+\varepsilon\big|\partial_t\xi^n_\alpha\big|_0^2\Delta t+M\Big\{\sum_{\alpha=1}^{n_c-1}\big|\xi^n_\alpha\big|_0^2+|||\sigma^{n+1}|||+h_p^4+h^4+(\Delta t)^2\Big\}\Delta t\\
&-(\Delta t)^3\Big\{\langle\delta_{\bar{x}}(D\delta_x(\phi^{-1}\delta_{\bar{y}}(D\delta_y(\partial_t\xi^n_\alpha)))),\partial_t\xi^n_\alpha\rangle+\langle\delta_{\bar{x}}(D\delta_x(\phi^{-1}\delta_{\bar{z}}(D\delta_z(\partial_t\xi^n_\alpha)))),\partial_t\xi^n_\alpha\rangle\\
&+\langle\delta_{\bar{y}}(D\delta_y(\phi^{-1}\delta_{\bar{z}}(D\delta_z(\partial_t\xi^n_\alpha)))),\partial_t\xi^n_\alpha\rangle\Big\}+(\Delta t)^4\langle\delta_{\bar{x}}(D\delta_x(\phi^{-1}\delta_{\bar{y}}(D\delta_y(\phi^{-1}\delta_{\bar{z}}(D\delta_z(\partial_t\xi^n_\alpha)))))),\partial_t\xi^n_\alpha\rangle.
\end{aligned}\tag{36}$$

Using the following fact

$$\hat{\xi}^n_{\alpha,ijk}-\xi^n_{\alpha,ijk}=\int_{X_{ijk}}^{\hat{X}^n_{ijk}}\nabla\xi^n_\alpha\cdot\mathbf{U}^{n+1}_{ijk}/\big|\mathbf{U}^{n+1}_{ijk}\big|ds,\ X_{ijk}\in\Omega_h,\tag{37a}$$

and eqs. (23), (33), we estimate the first term on the right-hand side of (36),

$$\Big|\sum_{\Omega_h}\phi_{ijk}\frac{\hat{\xi}^n_{\alpha,ijk}-\xi^n_{\alpha,ijk}}{\Delta t}\partial_t\xi^n_{\alpha,ijk}h^x_ih^y_jh^z_k\Big|\le\varepsilon\big|\partial_t\xi^n_\alpha\big|_0^2+M\big|\nabla_h\xi^n_\alpha\big|_0^2,\tag{37b}$$

where $\big|\nabla_h\xi^n_\alpha\big|_0^2=\sum_{s=x,y,z}\big|\partial_s\xi^n_\alpha\big|_0^2$.

Consider the fourth term in (36). Note that

$$\begin{aligned}
&-(\Delta t)^3\Big\{\langle\delta_{\bar{x}}(D\delta_x(\phi^{-1}\delta_{\bar{y}}(D\delta_y(\partial_t\xi^n_\alpha)))),\partial_t\xi^n_\alpha\rangle\\
&=-(\Delta t)^3\Big\{\langle\delta_x(D\delta_y(\partial_t\xi^n_\alpha)),\delta_y(\phi^{-1}D\delta_x(\partial_t\xi^n_\alpha))\rangle+\langle D\delta_y(\partial_t\xi^n_\alpha),\delta_y(\delta_x\phi^{-1}\cdot D\delta_x(\partial_t\xi^n_\alpha))\rangle\Big\}\\
&=-(\Delta t)^3\sum_{\Omega_h}\Big\{D_{i,j+1/2,k}D_{i+1/2,jk}\phi^{-1}_{ijk}[\delta_x\delta_y\partial_t\xi^n_{\alpha,ijk}]^2+[D_{i,j+1/2,k}\delta_y(D_{i+1/2,jk}\phi^{-1}_{ijk})\delta_x(\partial_t\xi^n_{\alpha,ijk})\\
&+D_{i+1/2,jk}\phi^{-1}_{ijk}\delta_xD_{i,j+1/2,k}\cdot\delta_y(\partial_t\xi^n_{\alpha,ijk})+D_{i,j+1/2,k}D_{i+1/2,jk}\delta_y(\partial_t\xi^n_{\alpha,ijk})]\cdot\delta_x\delta_y\partial_t\xi^n_{\alpha,ijk}\\
&+[D_{i,j+1/2,k}D_{i+1/2,jk}\delta_x\delta_y\phi^{-1}_{ijk}+D_{i,j+1/2,k}\delta_yD_{i+1/2,jk}\delta_x\phi^{-1}_{ijk}]\delta_x(\partial_t\xi^n_{\alpha,ijk})\delta_y(\partial_t\xi^n_{\alpha,ijk})\Big\}h^x_ih^y_jh^z_k.
\end{aligned}\tag{38}$$

Using the positive definiteness of D and the Cauchy inequality, and cancelling the high-order difference quotients $\delta_x\delta_y(\partial_t\xi^n_{\alpha,ijk})$, we estimate the first four terms in (38)

$$\begin{aligned}&-(\Delta t)^3\sum_{\Omega_h}\Big\{D_{i,j+1/2,k}D_{i+1/2,jk}\phi^{-1}_{ijk}[\delta_x\delta_y\partial_t\xi^n_{\alpha,ijk}]^2+[D_{i,j+1/2,k}\delta_y(D_{i+1/2,jk}\phi^{-1}_{ijk})\delta_x(\partial_t\xi^n_{\alpha,ijk})\\&+D_{i+1/2,jk}\phi^{-1}_{ijk}\delta_xD_{i,j+1/2,k}\cdot\delta_y(\partial_t\xi^n_{\alpha,ijk})+D_{i,j+1/2,k}D_{i+1/2,jk}\delta_y(\partial_t\xi^n_{\alpha,ijk})]\cdot\delta_x\delta_y\partial_t\xi^n_{\alpha,ijk}\Big\}h^x_ih^y_jh^z_k\\&\le M\Big\{\left|\nabla_h\xi^{n+1}_\alpha\right|_0^2+\left|\nabla_h\xi^n_\alpha\right|_0^2\Big\}\Delta t.\end{aligned}\tag{39a}$$

The last part in (38) is estimated,

$$\begin{aligned}&-(\Delta t)^3\sum_{\Omega_h}\Big\{[D_{i,j+1/2,k}D_{i+1/2,jk}\delta_x\delta_y\phi^{-1}_{ijk}+D_{i,j+1/2,k}\delta_yD_{i+1/2,jk}\delta_x\phi^{-1}_{ijk}]\delta_x(\partial_t\xi^n_{\alpha,ijk})\delta_y(\partial_t\xi^n_{\alpha,ijk})\Big\}h^x_ih^y_jh^z_k\\&\le M\Big\{\left|\nabla_h\xi^{n+1}_\alpha\right|_0^2+\left|\nabla_h\xi^n_\alpha\right|_0^2\Big\}\Delta t.\end{aligned}\tag{39b}$$

Similarly, we have the estimate of the fourth term in (36)

$$\begin{aligned}&-(\Delta t)^3\Big\{\langle\delta_{\bar x}(D\delta_x(\phi^{-1}\delta_{\bar y}(D\delta_y(\partial_t\xi^n_\alpha)))),\partial_t\xi^n_\alpha\rangle+\langle\delta_{\bar x}(D\delta_x(\phi^{-1}\delta_{\bar z}(D\delta_z(\partial_t\xi^n_\alpha)))),\partial_t\xi^n_\alpha\rangle\\&+\langle\delta_{\bar y}(D\delta_y(\phi^{-1}\delta_{\bar z}(D\delta_z(\partial_t\xi^n_\alpha)))),\partial_t\xi^n_\alpha\rangle\Big\}\\&\le M\Big\{\left|\nabla_h\xi^{n+1}_\alpha\right|_0^2+\left|\nabla_h\xi^n_\alpha\right|_0^2\Big\}\Delta t.\end{aligned}\tag{40}$$

The last term in (36) is argued by the Cauchy inequality and the treatment of $\delta_x\delta_y\delta_z(\partial_t\xi^n_{\alpha,ijk})$,

$$(\Delta t)^4\langle\delta_{\bar x}(D\delta_x(\phi^{-1}\delta_{\bar y}(D\delta_y(\phi^{-1}\delta_{\bar z}(D\delta_z(\partial_t\xi^n_\alpha)))))),\partial_t\xi^n_\alpha\rangle\le M\Big\{\left|\nabla_h\xi^{n+1}_\alpha\right|_0^2+\left|\nabla_h\xi^n_\alpha\right|_0^2\Big\}\Delta t.\tag{41}$$

Substituting (37), (40) and (41) into (36), we have

$$\begin{aligned}&\left|\partial_t\xi^n_\alpha\right|_0^2\Delta t+\frac12\sum_{s=x,y,z}\Big\{\langle D\delta_s\xi^{n+1}_\alpha),\delta_s\xi^{n+1}_\alpha\rangle-\langle D\delta_s\xi^n_\alpha),\delta_s\xi^n_\alpha\rangle\Big\}\\&\le\varepsilon\left|\partial_t\xi^n_\alpha\right|_0^2\Delta t+M\Big\{\left|\xi^n_\alpha\right|_0^2+\left|\nabla_h\xi^{n+1}_\alpha\right|_0^2+\left|\nabla_h\xi^n_\alpha\right|_0^2+|||\sigma^{n+1}|||^2+|\partial_t\pi^n|_0^2+h_p^4+h^4+(\Delta t)^2\Big\}\Delta t,\\&\quad\alpha=1,2,\cdots,n_c-1.\end{aligned}\tag{42}$$

Multiplying both sides of (29) by Δt, summing them on t $(0\le n\le L)$ and using $\pi^0=0$, we obtain

$$\begin{aligned}&\left\|\pi^{L+1}\right\|_m^2+\left|\left|\left|\sigma^{L+1}\right|\right|\right|^2+\sum_{n=0}^L\|\partial_t\pi^n\|_m^2\,\Delta t\le\varepsilon\sum_{n=0}^L\left\|\partial_t\xi^n\right\|_m^2\Delta t+\sum_{n=0}^L((d(C^n)-d(c^{n+1}))\pi^n.\pi^n)_m\Delta t\\&\quad+M\Big\{\sum_{n=0}^L[\left\|\pi^n\right\|_m^2+\sum_{\alpha=1}^{n_c-1}\left\|\xi^n_\alpha\right\|_m^2+\left|\left|\left|\sigma^n\right|\right|\right|^2]\Delta t+h_p^4+(\Delta t)^2\Big\}\\&\quad\le\varepsilon\sum_{n=0}^L\left\|\partial_t\xi^n\right\|_m^2\Delta t+M\Big\{\sum_{n=0}^L[\left\|\pi^n\right\|_m^2+\sum_{\alpha=1}^{n_c-1}\left\|\xi^n_\alpha\right\|_m^2+\left|\left|\left|\sigma^n\right|\right|\right|^2]\Delta t+h_p^4+(\Delta t)^2\Big\}.\end{aligned}\tag{43}$$

Sum (42) on α $(1\le\alpha\le n_c-1)$, multiply the resulting formulation by Δt, then make the sum on t $(0\le n\le L)$. By $\xi^0_\alpha=0,\alpha=1,2,\cdots,n_c-1$, it holds

$$\begin{aligned}&\sum_{n=0}^L\sum_{\alpha=1}^{n_c-1}\left|\partial_t\xi^n_\alpha\right|_0^2\Delta t+\frac12\sum_{\alpha=1}^{n_c-1}\sum_{s=x,y,z}\langle D\delta_s\xi^{L+1}_\alpha,\delta_s\xi^{L+1}_\alpha\rangle\\&\le M\sum_{n=0}^L\left|\partial_t\pi^n\right|\Delta t+M\Big\{\sum_{n=0}^L\Big[\sum_{\alpha=1}^{n_c-1}[\left|\xi^n_\alpha\right|_0^2+\left|\nabla_h\xi^{n+1}_\alpha\right|_0^2]+\left|\left|\left|\sigma^n\right|\right|\right|^2\Big]\Delta t+h_p^4+h^4+(\Delta t)^2\Big\}.\end{aligned}\tag{44}$$

Considering (43) and (44) together, and using the relation of different norms (Yuan, 1992, 1993; Douglas, 1982), we have

$$\begin{aligned}&\left\|\pi^{L+1}\right\|_m^2+\left|\left|\left|\sigma^{L+1}\right|\right|\right|^2+\sum_{n=0}^L\|\partial_t\pi^n\|_m^2\,\Delta t+\sum_{\alpha=1}^{n_c-1}[\left|\xi^{L+1}_\alpha\right|_0^2+\left|\nabla_h\xi^{L+1}_\alpha\right|_0^2]+\sum_{n=0}^L\sum_{\alpha=1}^{n_c-1}\left|\partial_t\xi^n_\alpha\right|^2\Delta t\\&\le M\Big\{\sum_{n=0}^L\Big[\|\pi^n\|_m^2+\left|\left|\left|\sigma^n\right|\right|\right|^2+\sum_{\alpha=1}^{n_c-1}[\left|\xi^n_\alpha\right|_0^2+\left|\nabla_h\xi^{n+1}_\alpha\right|_0^2]\Big]\Delta t+h_p^4+h^4+(\Delta t)^2\Big\}.\end{aligned}\tag{45}$$

Using $\xi_\alpha^0 = 0$, $\left|\xi_\alpha^{L+1}\right|_0^2 \le \varepsilon \sum_{n=0}^{L} \left|\partial_t \xi_\alpha^n\right|_0^2 \Delta t + K \sum_{n=0}^{L} \left|\xi_\alpha^n\right|_0^2 \Delta t$, and the Gronwall Lemma, we have

$$\begin{aligned}&\left\|\pi^{L+1}\right\|_m^2 + \left|\left|\left|\sigma^{L+1}\right|\right|\right|^2 + \sum_{n=0}^{L} \|\partial_t \pi^n\|_m^2 \Delta t + \sum_{\alpha=1}^{n_c-1} [\left|\xi_\alpha^{L+1}\right|_0^2 + \left|\nabla_h \xi_\alpha^{L+1}\right|_0^2] + \sum_{n=0}^{L}\sum_{\alpha=1}^{n_c-1} \left|\partial_t \xi_\alpha^n\right|^2 \Delta t \\ &\le M\left\{h_p^4 + h^4 + (\Delta t)^2\right\}.\end{aligned} \tag{46}$$

It remains to testify the induction hypothesis (23). From the initial conditions, $\eta^0 = 0$, $\xi_\alpha^0 = 0, \alpha = 1, 2, \cdots, n_c - 1$ and $\rho = 0$, (23) holds obviously for $n = 0$. If it is right for $1 \le n \le L$, then by (46) and (33), we have

$$\sum_{\alpha=1}^{n_c-1} \left\|\xi_\alpha^{L+1}\right\|_\infty \le Mh^{-3/2}\left\{h_p^2 + h^2 + \Delta t\right\} \le Mh_p^{1/2} \to 0, \tag{47}$$

$$\left|\left|\left|\sigma^{L+1}\right|\right|\right|_\infty \le Mh^{-3/2}\left\{h_p^2 + h^2 + \Delta t\right\} \le Mh_p^{1/2} \to 0, \tag{48}$$

Thus, it holds for $n = L + 1$.

Theorem 1. *Suppose that the problem of (1) and (2) is regular (R) and positive definite (C). The composite scheme of (13), (14)-(16) and (17) is applied. Under the restriction (33), it holds*

$$\begin{aligned}&\|p - P\|_{\bar{L}^\infty(J;L^2(\Omega))} + \|\partial_t(p - P)\|_{\bar{L}^2(J;L^2(\Omega))} + \|\mathbf{u} - \mathbf{U}\|_{\bar{L}^\infty(J;V)} + \sum_{\alpha=1}^{n_c-1} \|c_\alpha - C_\alpha\|_{\bar{L}^\infty(J;l^2(\Omega))} \\ &+ \sum_{\alpha=1}^{n_c} \|\nabla_h(c_\alpha - C_\alpha)\|_{\bar{L}^\infty(J;l^2(\Omega))} + \sum_{\alpha=1}^{n_c} \|\partial_t(c_\alpha - C_\alpha)\|_{\bar{L}^2(J;l^2(\Omega))} \\ &\le M^*\left\{h_p^2 + h^2 + \Delta t\right\},\end{aligned} \tag{49}$$

where $\|g\|_{\bar{L}^\infty(J;X)} = \sup_{n\Delta t \le T} \|g^n\|_X$, $\|g\|_{\bar{L}^2(J;X)} = \sup_{L\Delta t \le T} \{\sum_{n=0}^{L} \|g^n\|_X^2 \Delta t\}^{1/2}$*, and the constant* M^* *depends on* p, c_α $(\alpha = 1, 2, \cdots, n_c)$ *and their derivatives.*

6. Conclusions and Discussions

In this paper, the authors present a mixed volume element modified with characteristic fractional step difference, and discuss its numerical analysis. The mathematical model, physical interpretation and academic research are introduced in §1. Two different partitions (coarse and refined) are given for defining the scheme, and some preliminary properties are stated for theoretical analysis in §2. In §3, the authors formulate the procedures based on the combination of the mixed volume element and modified characteristic fractional step difference. The mixed volume element has the conservative nature for the flow. The characteristic fractional step difference is illustrated to compute the concentration vector without numerical oscillations. A large time step is adopted and the speedup algorithm is used during the whole computation. The three-dimensional work is accomplished effectively by solving three successive one-dimensional problems. In §4, using the variation, energy norm analysis, the usage of different meshes, piecewise product threefold quadratic interpolation, decomposition of high-order difference operators and the interchangeability of different operators, we obtain an optimal error estimates in L^2-norm. There are several interesting conclusions.

- This discussion considers the compressibility and the multicomponent, thus the numerical simulation is possibly consistent with the truth.
- The composite procedures could be carried out in three-dimensional complicated region.
- The mixed volume element has the nature of conservation, and improves the computational accuracy of Darcy one order. This property is important in numerical simulation of two-phase seepage displacement.
- The concentration vector is computed by the characteristic fractional step difference, where a large time step is used and second accuracy is preserved. Thus, this parallel algorithm could be carried out to complete numerical simulation on parallel computers.

Acknowledgements

This work is supported by the Natural Science Foundation of Shandong Province (Grant No. ZR2021MA019).

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